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Finite-Difference Fluid Dynamics Computer Mathematical Models for the Design and Interpretation of Experiments for Space Flight

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NASA

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TECHNICAL PAPER

FINITE-DIFFERENCE FLUID DYNAMICS COMPUTER MATHEMATICAL MODELS FOR THE DESIGN AND INTERPRETATION OF EXPERIMENTS FOR SPACE FLIGHT

I. INTRODUCTION

Spacelab flights using NASA's Space Shuttle have begun and regular flights are planned for the future. Among other uses, Spacelab has been designed to exploit the microgravity environment of an orbiting vehicle for science and technology. In particular, there are many basic fluid dynamics experiments, and materials processing studies involving fluid motions, which can only achieve their full potential in a low-gravity environment. NASA has also proposed to build a space station for which low-gravity experimentation will be a major application. This paper deals with three fluid dynamical experiments which are under consideration for space flight and with the computer mathematical models which are being developed and used for the design and interpretation of these experiments.

Recent advances in numerical modeling methods and the continued improvement in computing speed and memory are opening up a new era for theoretical physics and engineering. In particular, accurate numerical models of non-turbulent, incompressible fluid flows in simple geometries can now be developed in a systematic manner. Sufficient numerical methods and numerical stability criteria are known so that this is no longer an art. Further, when accurate and detailed data are required for a fluid dynamical problem, numerical modeling is often the only procedure available. Nonseparability and non-linearity of the governing differential equations can make it impossible to use analytical methods, and the properties of many fluids and thin boundary layers can make it very difficult to use experimental methods. When such difficulties arise, the following procedure has been used to solve the problem [1,2]. First, develop a computer code and build an apparatus for the flow to be investigated. Then check the code predictions using data from relatively simple but significant measurements made with the apparatus. To obtain good agreement, it may be necessary to adjust some of the code control parameters, such as the space and time resolutions. Once validated, the code alone can be used to obtain accurate and detailed data about the flow over the range of validation. (There may also be occasions when a code can be validated using theoretical results over their range of validity.)

The constraints and high cost of space flight experimentation mean that quantitative design studies should be performed. The procedure outlined previously is well suited to the design and interpretation of such experiments. Clearly, the validation method cannot now be carried out directly. However, results from one or more similar laboratory experiments which deal with the physical processes involved can be used instead to check the code. This procedure is being used to design a spherical baroclinic flow model experiment of the large-scale atmosphere flow for Spacelab and to study the processes at work in crystal growing systems which are also candidates for space flight.

II. THE ATMOSPHERIC GENERAL CIRCULATION EXPERIMENT

A. Experiment

A substantial amount of research into large-scale baroclinic atmospheric dynamics has been performed using a laboratory cylindrical annulus model [3]. The microgravity environment of Spacelab presents the opportunity to realize a true spherical-layer model. Such an experiment, known as the

Atmospheric General Circulation Experiment (AGCE), has been proposed to NASA for Spacelab flights. In the AGCE radial gravity is simulated by a dielectric body force, which is only dominant in the absence of ordinary gravity. The AGCE has been described elsewhere [4,5,6] and a substantial number of scientific support studies have been performed [7-13]. A spherical convection experiment known as the Geophysical Fluid Flow Cell which also uses the radial dielectric body force will be flown on Spacelab 3 [14]. Proposed configurations for the AGCE are shown in Figure 1. For quantitative design studies numerical models are required, and a numerical design studies program is well underway [15,6]. The most important design criterion is that baroclinic instability be realized in the apparatus.
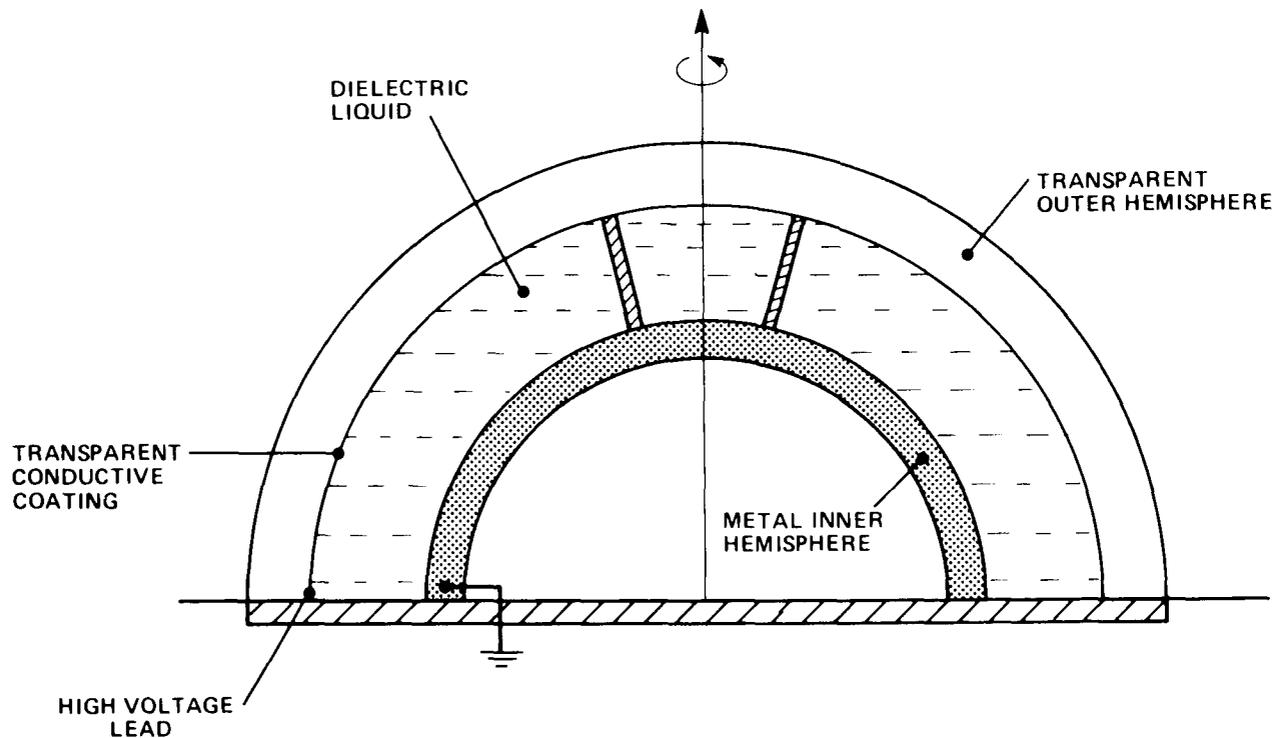

Figure 1. Schematic drawing of the proposed AGCE apparatus. The high latitude boundary will be used if a hemispherical annulus configuration is selected.

B. Numerical Models

To determine in parameter space the baroclinically unstable region for the AGCE, two finite-difference codes have been developed. The first solves the axisymmetric Navier-Stokes equations in spherical coordinates to obtain basic states. The second uses the linearized, three-dimensional Navier-Stokes equations to examine these basic states for instabilities with azimuthal structure. Detailed descriptions of these two codes have been given by Fowlis and Roberts [6]. Only a very brief description is given here.

With appropriate choices for the geometrical control parameters, we can calculate basic state flows in a spherical or hemispherical layer, or in a sphere. Boundaries can be introduced at any latitude. We can also approximate a cylinder or a cylindrical annulus by choosing a very large inner radius and a limited latitudinal range from the axis of symmetry for the latitudinal boundaries. A wide range of boundary conditions (e.g., no flow, stress free, insulating, and conducting) is available. Nonuniform meshes and implicit iterative methods are used. The iterative method for steady solutions is based on

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time-stepping but has the options of different time steps for velocity and temperature and of a time step varying smoothly with position according to specified powers of the mesh spacings. This allows for more rapid convergence. The linear azimuthal wave stability equations are solved by an iterative method which corresponds closely with the axisymmetric method.

Validation of the axisymmetric code using data from previous work in cylindrical geometry was described in Reference 6. To check the spherical terms we compared the code predictions for spin-up in a homogeneous sphere of fluid [16] with laser-Doppler measurements of this flow [17]. Good agreement was obtained. To validate the stability code, it was applied to the computations of basic state flows in a rotating cylindrical annulus. Good agreement was obtained with the experimental results of Fowlis and Hide [18]. A parallel research effort, in which a similar code was used and approximately the same agreement obtained, has been published by Miller and Gall [13]; their results are shown in Figure 2.
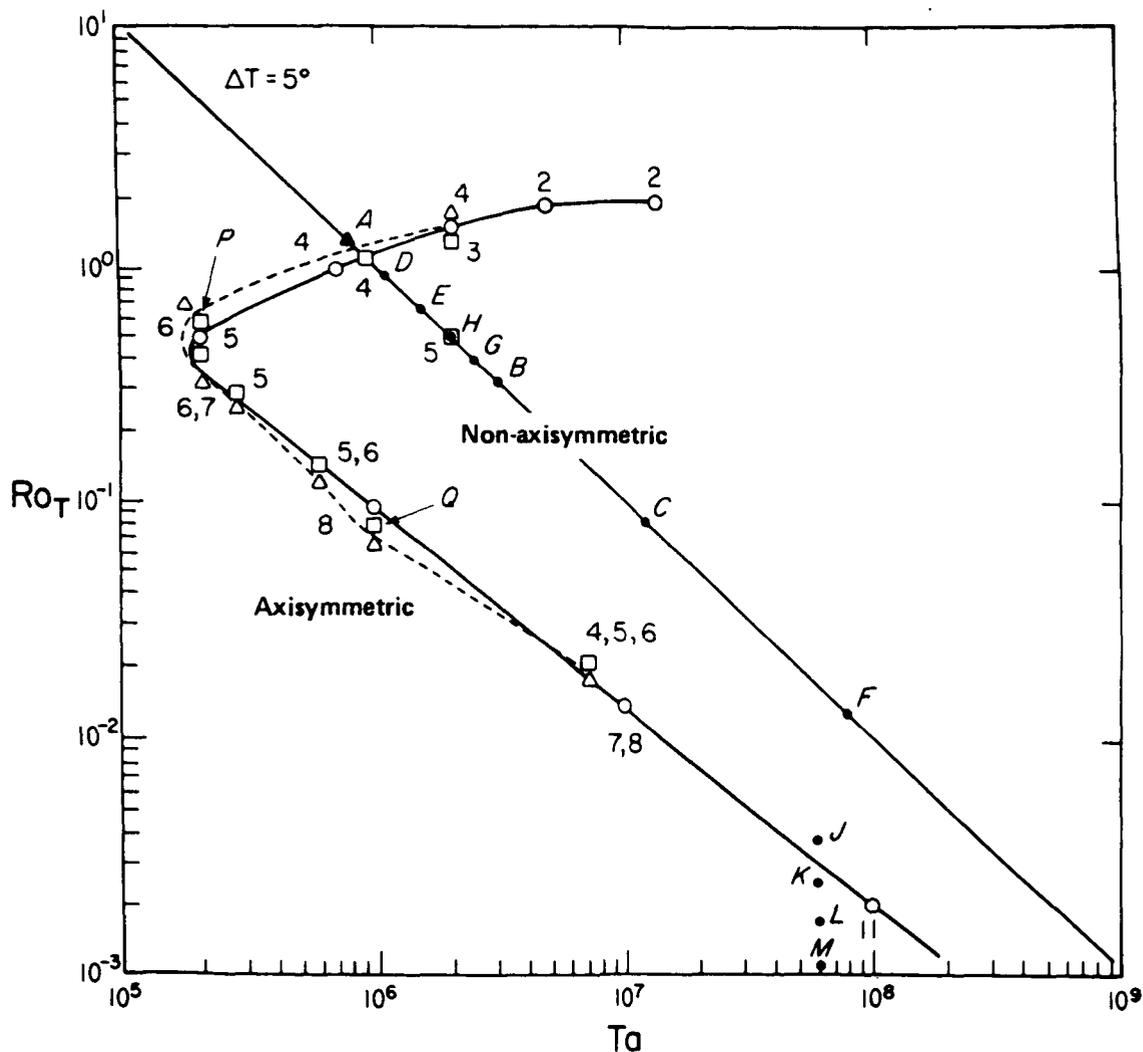

Figure 2. A comparison of experimental and numerical results for the regime diagram for the baroclinic cylindrical annulus flows taken from Miller and Gall [13]. The experimental results for marginal stability are shown by the continuous curve and the numerical results by the dashed curve. Further details can be found in the paper.

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In further support of the AGCE program, a fully nonlinear, three-dimensional code is being developed. This code uses the same spherical-layer geometry and allows for the same geometrical options as before. It is designed to compute either steady states, using the same techniques as before for rapid convergence, or time-dependent solutions. The primitive variables are used on a nonuniform, staggered computational mesh. Advection, diffusion, the Coriolis force, and internal waves are all handled implicitly, to reduce or eliminate the corresponding limitations on the time step. This code will be validated using known wave flows in the cylindrical annulus. It is important to have prior estimates of the amplitude and structure of the wave flows to be expected in the AGCE. The code will be used both for design of the AGCE and later for interpreting actual AGCE flows.

C. Results

A definite configuration for the AGCE in terms of latitudinal boundaries, radial depth, boundary temperature distributions, and fluid properties is not yet settled; such specifications should come out of the design studies. Figure 1 shows a hemispherical-layer configuration, which can be heated and cooled at the equatorial and high latitude boundaries, respectively, similar to the cylindrical annulus. We are computing the regime diagram for such a spherical annulus configuration, and the results to date are shown in Figure 3. At this point, the results suggest that the diagram will be very different from the cylindrical annulus diagram shown in Figure 2.
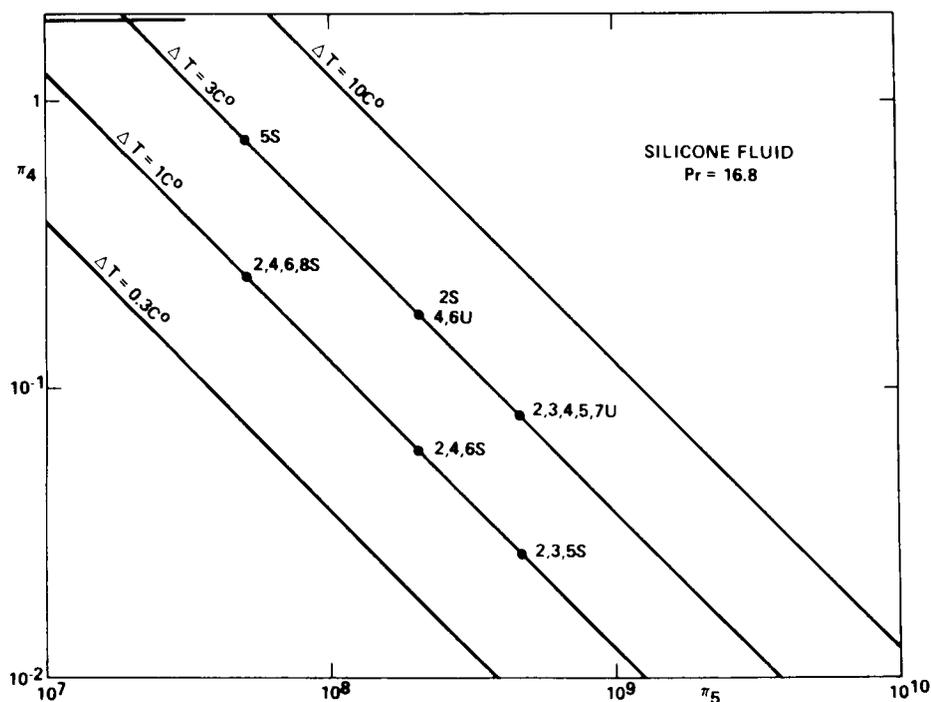
Figure 3. Preliminary regime diagram for the hemispherical-layer annulus configuration. The azimuthal wavenumbers are shown, and whether they were found to be stable (S) or unstable (U) is also indicated. The results are shown as a plot of $\pi_4 (\equiv \alpha g D \Delta T / \Omega^2 L^2)$ versus $\pi_5 (\equiv 4\Omega^2 L^5 / \nu^2 D)$ for a fixed value of Pr ($\equiv \nu/\kappa$), where D is the radial fluid depth, L the latitudinal extent, α the coefficient of cubical expansion, ν the kinematic viscosity, κ the thermal diffusivity, ΔT the imposed latitudinal temperature difference, and Ω the rotation rate. For these results the inner radius = 4.5 cm, the outer radius = 6.5 cm, and the high latitude boundary was located at 0.45 radians from the polar axis. The liquid was silicone fluid with ν = 0.01 cm^2/s.

Problems are being experienced with slow convergence of the algorithm which computes the fastest growing (or slowest decaying) eigenmode for linear disturbances to the basic state. The algorithm is related to time-stepping the evolution equations, but with a time step which varies with position and for different variables. This attempt to obtain rapid convergence has been successful for a large number of cases, particularly in an annular geometry. However, it has not been as successful for most of the spherical-layer geometry cases analyzed. Therefore, small time steps with correspondingly slow convergence must be used.

III. CONVECTION IN A FLOAT ZONE

A. The Float Zone System

In the float zone process of crystal growth, a ring heater maintains a small zone of liquid melt between a polycrystalline feed rod and a rod of single crystal. The small volume of liquid is held in place by surface tension. The feed rod is moved into the zone where it melts, while the other rod is pulled out of the zone resulting in growth as a single crystal. In order to achieve desired properties for the crystal, the liquid melt is usually made up of two or more different substances. Ideally, the components should be distributed uniformly throughout the crystal. However, in general, this is very difficult to achieve [19]. The variation of component concentration in the crystal is caused by the flow and temperature fields in the melt. Strong flows can also cause crystal imperfections with a single component. Since buoyancy-driven flows are suppressed in the absence of gravity, float zone systems are candidates for space flight. However, even in the absence of gravity, the variation of surface tension with temperature on the free surface will drive motions.

As a first step in understanding the interaction between the flow and temperature fields and the crystallization process, Smith and Greenspan [20] investigated the motions occurring in the float zone in the absence of crystal growth. These workers added rotation to examine its influence in confining the flows to boundary layers. Adding rotation also adds another driving force, centrifugal buoyancy. Smith and Greenspan examined, separately, the flows driven in a rotating cylinder of fluid by thermocapillary and centrifugal buoyancy forces. Ordinary gravity was neglected. These workers used analytical methods and linearized equations. They considered a melt zone which was hot at one end and cold at the other. Using numerical methods, this model is extended to the nonlinear case; and, using both analytical and numerical methods, the more realistic model with a temperature distribution symmetrical about mid-depth is examined.

B. The Numerical Model

For this work, the axisymmetric code already developed for the AGCE basic state studies can be used (see Section II). The conversion to cylindrical geometry was again carried out by letting the radius of the inner sphere be very large and considering only a small latitude range from the axis of symmetry. The stress boundary conditions at the outer cylindrical surface were changed to implement the thermocapillary boundary condition (temperature-dependent surface tension).

C. Results

Following Smith and Greenspan [20], thermocapillary-driven flow and the centrifugal buoyancy-driven flow were considered separately. Smith and Greenspan presented results for a cylinder of silicon liquid (for details see Figure 4 caption). They found, for the linearized problem, that the flow driven

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by the temperature variation of surface tension at the free outer cylindrical surface is confined to a boundary layer on that surface and that there is no flow in the interior. However, Smith and Greenspan noted that the dimensionless parameter determining the strength of the nonlinear terms was not small for the case they considered. Their case was repeated using the fully nonlinear numerical model and it was found that the boundary layer flow forces its way into the interior. The stream function is shown in Figure 4. Additional computation showed that for this case there is little difference between the rotating and the nonrotating flows. However, the suggestion to use rotation to limit the extent of the flow may still be useful if a suitable surfactant, to reduce the thermocapillary effect, can be found.

This paper does not present the rest of the results on float zone convection. These results should be published soon [21].
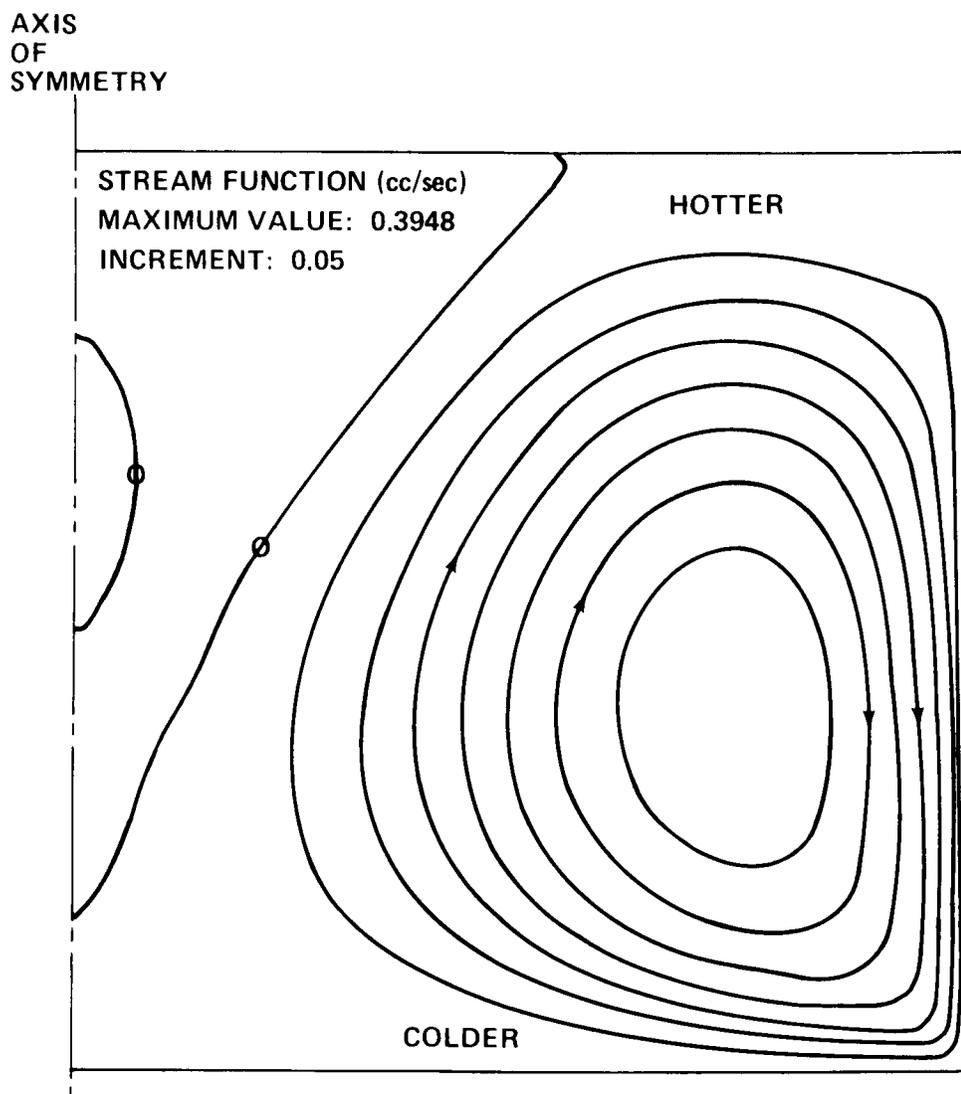
Figure 4. Flow in a rotating float zone driven only by surface tension variation in the outer cylindrical boundary. Contours of the stream function are plotted. The results are for: radius = 1 cm, height = 1 cm, vertical temperature difference = 5°C, and rotation = 1 rad/s. The fluid was liquid silicon with surface tension = 720 dyne/cm, surface tension temperature coefficient = -0.43 dyne/cm C°, kinematic viscosity = 0.0035 cm^2/s, and thermal diffusivity = 0.15 cm^2/s. The maximum value for the vertical (axial) flow at the surface was about 25 cm/s.

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IV. THE BRIDGMAN-STOCKBARGER CRYSTAL GROWING SYSTEM

A. The Bridgman-Stockbarger Configuration

The Bridgman-Stockbarger system is one of the most widely used methods for growing crystals in the laboratory. In this method, a cylindrical ampoule containing the liquid melt is lowered steadily from a hot isothermal container into a relatively cooler container. Solidification begins at the bottom of the ampoule and proceeds upwards as the ampoule is withdrawn. Again as for the float zone system, to achieve desired properties for the crystal, the liquid usually consists of two or more different substances. Although the Bridgman-Stockbarger system has been used successfully to produce crystals for many applications, there are also many cases where the full potential of the crystalline material is not achieved for the reasons already given in Section III.

The temperature and flow fields influence the crystal growth in two ways. First, they can affect the shape of the solidification interface which in turn can affect the radial concentration of the melt components. Second, the flow field can modify the thickness of the diffusion boundary layers of component-rich liquid which form near the solidification interface, as a result of differential segregation of the components during solidification. This thickness modification then affects the concentrations of the melt components incorporated into the crystal.

A fuller understanding of the physical processes at work in this system would almost certainly lead to improvements in the crystals produced, and a numerical modeling effort appears to be a worthwhile approach. For many cases of practical interest, experimental measurement and observation are difficult or impossible, since the substances are metals at elevated temperatures and pressures. Analytical approaches are hindered by the complex geometry and by the nonlinearity and instability of the flows.

B. Numerical Model

A code is being developed to compute time-dependent and steady state axisymmetric solutions for the Bridgman-Stockbarger system. The code will be flexible, to describe a variety of geometries, materials, and thermal configurations, for laboratory and industrial applications and for space.

The temperature equation is solved in the liquid, the solid, and the ampoule, using flexibly-defined thermal forcing on the boundaries and using appropriate interface conditions including latent heat release. The concentration equation for a secondary component and the equations of motion are solved in the melt. An incompressible Boussinesq fluid, with the buoyancy in general a function of both the temperature and concentration, and with an imposed density (and volume) change on solidification is assumed.

The code uses a nonuniform mesh defined using a coordinate transformation, so that the unknown interface is a coordinate surface. The radial mesh is also nonuniform. The interface height is a function of radius and time; its evolution is determined using an implicit representation of the interface conditions, based on the equations of state.

The heat equation is time-stepped using an implicit method. For typical applications, the thermal conductivities are very large, and this implicit method essentially amounts to a separate solution of the steady state problem at every time step. The concentration equation is also time-stepped by an implicit method. Here the diffusivity is very low, and this method is normally required only if the flow is rapid and the advection stability criterion would otherwise be violated.

The equations of motion are solved using a vorticity and stream function formulation, with viscosity, advection, Coriolis force, and internal waves all treated implicitly. Again, this is required because the time step would otherwise have to be very small. The Bridgman-Stockbarger system will require prolonged calculations. Model predictions will be compared with laboratory measurements made using different Bridgman-Stockbarger systems by our colleagues in the Space Science Laboratory at Marshall Space Flight Center (S. L. Lehoczky, D. O. Frazier, F. R. Szofran, and D. Chandra).

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16. ABSTRACT

A major objective of NASA's Spacelab is to exploit the microgravity environment of an orbiting vehicle for science and technology. There are many fundamental fluid dynamics experiments and materials processing studies involving fluid motions which can only achieve their full potential in a low-gravity environment. The many constraints and high costs of space experimentation mean that quantitative and detailed scientific and engineering design studies should be performed before proceeding to the construction of flight apparatus. However, for experiments involving fluid dynamics, such studies are not easily performed. Analytical methods are severely limited in their range of applicability by fundamental mathematical difficulties. Experimental measurement cannot, in principle, be performed until the apparatus is built and flown, but even laboratory analogs can present substantial difficulties to a detailed measurement program. The solution to the above difficulties can often be found in numerical modeling. Recent advances in numerical modeling methods mean that accurate numerical models for many fluid flow problems can now be developed in a systematic manner, and the continued improvement in computer hardware means that these models can be run in a relatively short time. In particular, models of non-turbulent, incompressible fluid flows in simple geometries can be developed to provide accurate and detailed data.

Numerical methods are used to design a spherical baroclinic flow model experiment of the large-scale atmosphere flow for Spacelab. The dielectric simulation of radial gravity is only dominant in a low-gravity environment. Computer codes are developed to study the processes at work in crystal growing systems which are also candidates for space flight. Crystalline materials rarely achieve their potential properties because of imperfections and component concentration variations. Thermosolutal convection in the liquid melt can be the cause of these imperfections. Such convection is suppressed in a low-gravity environment.

Two- and three-dimensional finite-difference codes are being used for this work. Nonuniform meshes and implicit iterative methods are used. The iterative method for steady solutions is based on time-stepping but has the options of different time steps for velocity and temperature and of a time step varying smoothly with position according to specified powers of the mesh spacings. This allows for more rapid convergence. The code being developed for the crystal growth studies allows for growth of the crystal at the solid-liquid interface. The moving interface is followed using finite differences; shape variations are permitted. For convenience in applying finite differences in the solid and liquid, a time-dependent coordinate transformation is used to make this interface a coordinate surface.

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